

Compactness of the set of Faddeev and Lippmann–Schwinger equations for the three-body Coulomb problem

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The set of Faddeev and Lippmann–Schwinger integral equations for three-body systems involving Coulomb interactions deduced from a “three-potential” picture are shown to be compact for all energies and a method of solution is given.

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There are two well-known, practical but genuinely different approaches to solve three-body scattering equations of Faddeev type and which involve Coulomb-like interactions. In the first of these, the Alt–Grassberger–Sandhas (AGS) equations are solved by the “screening and renormalizing” technique. This approach and its applications are discussed in a recent review [1]. The alternative approach is to solve the Faddeev–Noble differential equations. To do so, in configuration space, one needs asymptotic boundary conditions. This approach has also been reviewed recently [2]. Although these approaches have been in use for some time, problems still exist with the renormalization procedure of method one and with the approximate boundary condition required in method two. Consequently, to date, only limited solutions are available below or above the breakup threshold.

Herein I propose a new approach for solving the three-body Coulomb scattering problem. As usual, one presumes that the quantum mechanical system evolves from a state governed by the asymptotic Hamiltonian to the physical state described by the total Hamiltonian. In the two-potential formalism of that, an intermediate Hamiltonian must be defined and connection made first to the asymptotic Hamiltonian and then to the total Hamiltonian. The two-potential picture is a direct consequence of Kato’s chain rule for wave operators [3], which holds even for Coulomb interactions [4]. In a “three-potential” picture [5] a three-body Coulomb scattering process can be viewed as three consecutive scattering processes by which the asymptotic channel Hamiltonian connects to the total one via two intermediate Hamiltonians. This process can be formulated in terms of a set of the Faddeev and Lippmann–Schwinger integral equations. Numerically, these integral equations can be solved by using a Coulomb–Sturmian space representation. Hereafter I designate both the representation and the method by the label CS. The (CS) method has been used before and it has worked very well for bound-state problems with repulsive [6] and with attractive [7] Coulomb interactions. It has also been used to analyze $p-d$ scattering at energies below breakup [5] and the results agree very well with those obtained from other calculations [8].

In this article, I seek to extend the scope of this novel (CS) method to energies above the breakup threshold. I shall show that the Faddeev and Lippmann–Schwinger integral equations deduced from a “three-potential” picture by applying Kato’s chain rule possess compact kernels and so have unique solutions to the three-body Coulomb problem for all energies. I will also show how one can calculate the Green’s operator which contains all the asymptotically relevant terms for arbitrary complex energies.

I assume that the subsystem interaction, v_α , of two elements in a three-body system is a Coulomb-like one, which is then split into short-range and long-range terms as

$$v_\alpha(\xi_\alpha) = v_\alpha^{(s)}(\xi_\alpha) + v_\alpha^{(l)}(\xi_\alpha). \quad (1)$$

Here α denotes the subsystem and superscripts s and l indicate the short- and long-range attributes, respectively, with ξ_α and η_α being the usual configuration space Jacobi coordinates. The splitting should be performed in such a way that $v_\alpha^{(l)}$ does not support any bound states. The total Hamiltonian is denoted by H and the asymptotic channel Hamiltonian is defined by

$$H_\alpha = h_{\xi_\alpha}^0 + h_{\eta_\alpha}^0 + v_\alpha = H^0 + v_\alpha, \quad (2)$$

where h^0 and H^0 are the two-body and the three-body kinetic energy operators respectively. The asymptotic state $|\Phi_\alpha\rangle$ is an eigenstate of H_α , i.e.

$$H_\alpha|\Phi_\alpha\rangle = E_\alpha|\Phi_\alpha\rangle, \quad (3)$$

where $\langle\xi_\alpha\eta_\alpha|\Phi_\alpha\rangle = \langle\eta_\alpha|\chi_\alpha\rangle\langle\xi_\alpha|\phi_\alpha\rangle$ is a product of a continuum state in coordinate η_α and a bound or continuum state in the two-body subsystem ξ_α . If ϕ_α is a bound eigenstate, asymptotically there is a two-fragment channel. If it is a scattering state, the asymptote is a three-fragment channel. The scattering state, Ψ_α , which evolves from the asymptotic state, is given by applying the $\Omega^{(\pm)}(H, H_\alpha)$ Møller operators onto the asymptotic state

$$|\Psi_\alpha^{(\pm)}\rangle = \Omega^{(\pm)}(H, H_\alpha)|\Phi_\alpha\rangle. \quad (4)$$

The Møller operators are defined by the limit

$$\Omega^{(\pm)}(H, H_\alpha) = \lim_{t \rightarrow \mp\infty} \exp[iHt] \exp[-iH_\alpha(t)], \quad (5)$$

where $H_\alpha(t) = H_\alpha t + A(t)$ with $A(t)$ being the Dollard's distortion operator [9].

In the spirit of Kato's chain rule, I introduce two intermediate Hamiltonians, the channel long-range Hamiltonian

$$H_\alpha^{(l)} = H_\alpha + v_\beta^{(l)} + v_\gamma^{(l)}, \quad (6)$$

and the channel distorted long-range Hamiltonian

$$\tilde{H}_\alpha = H_\alpha + u_\alpha^{(l)}. \quad (7)$$

The auxiliary potential $u_\alpha^{(l)} = u_\alpha^{(l)}(\eta_\alpha)$ is defined such that it does not support any bound states and has the asymptotic form $u_\alpha^{(l)} \sim e_\alpha(e_\beta + e_\gamma)/\eta_\alpha$ as $\eta_\alpha \rightarrow \infty$. In fact, $u_\alpha^{(l)}$ is an effective Coulomb interaction between the center of mass of the subsystem α (with charge $e_\beta + e_\gamma$) and the third particle (with charge e_α). Now, according to Kato's chain rule the Møller operator (5) can be written in the form

$$\begin{aligned} \Omega^{(\pm)}(H, H_\alpha) &= \Omega^{(\pm)}(H, H_\alpha^{(l)}) \\ &\times \Omega^{(\pm)}(H_\alpha^{(l)}, \tilde{H}_\alpha) \Omega^{(\pm)}(\tilde{H}_\alpha, H_\alpha). \end{aligned} \quad (8)$$

The last term, $\Omega^{(\pm)}(\tilde{H}_\alpha, H_\alpha)$, which essentially describes a two-body scattering in the Coulomb-like potential $u_\alpha(\eta_\alpha)$, exists in Dollard's sense, and by applying it to the channel state gives

$$|\tilde{\Phi}_\alpha^{(\pm)}\rangle = \Omega^{(\pm)}(\tilde{H}_\alpha, H_\alpha)|\Phi_\alpha\rangle = |\tilde{\chi}_\alpha^{(\pm)}\rangle|\phi_\alpha\rangle \quad (9)$$

with $\langle\eta_\alpha|\tilde{\chi}_\alpha^{(\pm)}\rangle$ being a scattering solution in the Coulomb-like potential $u_\alpha^{(l)}$.

Now I will show that the middle term in (8) exists in the ordinary sense [10]

$$\Omega^{(\pm)}(H_\alpha^{(l)}, \tilde{H}_\alpha) = \lim_{t \rightarrow \mp\infty} \exp[iH_\alpha^{(l)}t] \exp[-i\tilde{H}_\alpha t]. \quad (10)$$

The necessary condition for the existence of the strong limit in (10) is that the potential

$$U^\alpha = H_\alpha^{(l)} - \tilde{H}_\alpha = v_\beta^{(l)} + v_\gamma^{(l)} - u_\alpha^{(l)} \quad (11)$$

should decrease in configuration space more rapidly than does the Coulomb potential [11]. Indeed, the auxiliary potential $u_\alpha^{(l)}$ has been constructed so that it cancels the long-range potentials $v_\beta^{(l)} + v_\gamma^{(l)}$ in U^α for the two-fragment channel α in which the particle labeled with α is in continuum state, while the particles labeled by β and γ form a bound state. Also, in the three-fragment channel of H_α , where the particles labeled by β and γ are in continuum state, U^α decreases with radius faster than

does the Coulomb potential. The term U^α would behave like a Coulomb potential in the two-fragment channels, β and γ , where particles α and γ or α and β form bound clusters, but for $H_\alpha^{(l)}$ there are no two-fragment channels β and γ .

Applying $\Omega^{(\pm)}(H_\alpha^{(l)}, \tilde{H}_\alpha)$ to the “free” state $|\tilde{\Phi}_\alpha^{(\pm)}\rangle$ yields

$$|\Phi_\alpha^{(l)(\pm)}\rangle = \Omega^{(\pm)}(H_\alpha^{(l)}, \tilde{H}_\alpha)|\tilde{\Phi}_\alpha^{(\pm)}\rangle. \quad (12)$$

Sandhas has shown in Ref. [12], that if for a three-body system only one of the potentials supports bound states, no rearrangement channels are possible, and therefore a single Lippmann–Schwinger equation is completely sufficient to guarantee the uniqueness of the solution. The Hamiltonian $H_\alpha^{(l)}$ possesses this property, thus the Lippmann–Schwinger integral equation which is derived from (10),

$$|\Phi_\alpha^{(l)(\pm)}\rangle = |\tilde{\Phi}_\alpha^{(\pm)}\rangle + \tilde{G}_\alpha(E_\alpha \pm i0)U^\alpha|\Phi_\alpha^{(l)(\pm)}\rangle, \quad (13)$$

with $\tilde{G}_\alpha(z) = (z - \tilde{H}_\alpha)^{-1}$, provides unique solution for this auxiliary three-body system. Additionally, Eq. (13) possesses a compact kernel because in the asymptotically accessible region, channel α , \tilde{G}_α is linked solely to the asymptotic behavior of $|\Phi_\alpha^{(l)(\pm)}\rangle$, and the source term, U^α , is of shorter range than the Coulomb interaction. Thus, in this particular Lippmann–Schwinger equation U^α can be approximated by finite rank terms. Note, that a similar equation holds for $G_\alpha^{(l)} = (z - H_\alpha^{(l)})^{-1}$:

$$G_\alpha^{(l)} = \tilde{G}_\alpha + \tilde{G}_\alpha U^\alpha G_\alpha^{(l)}. \quad (14)$$

Finally, $\Omega^{(\pm)}(H, H_\alpha^{(l)})$, which also exists in the usual sense, leads to the Faddeev–Noble integral equations [13],

$$|\psi_\beta^{(\pm)}\rangle = \delta_{\beta\alpha}|\Phi_\alpha^{(l)(\pm)}\rangle + G_\beta^{(l)}(E_\alpha \pm i0)v_\beta^{(s)} \sum_{\gamma \neq \beta} |\psi_\gamma^{(\pm)}\rangle, \quad (15)$$

where α, β, γ form a cyclic permutation. Merkuriev has shown that the kernels of these equations are compact for all energies [14], and thus the potential operators can be approximated well by finite rank terms. So, the set of Lippmann–Schwinger and Faddeev–Noble integral equations derived from a “three-potential” picture for the three-body Coulomb scattering problem, are uniquely solvable and possess compact kernels for all energies.

In this derivation a crucial point is that one Lippmann–Schwinger equation of the type given in Eq. (13) suffices for a unique solution to be found. This is the case if one imposes a condition on $v^{(l)}$ that it should not support bound states. This condition is satisfied if all the Coulomb interactions in the three-body system are repulsive. With a three-nucleon system then, one would take

$v_\alpha^{(s)}$ as the nuclear potential and $v_\alpha^{(l)}$ as the Coulomb interaction. The situation is more complicated if some of the Coulomb interactions are attractive. There are an infinite number of bound states associated with an attractive Coulomb potential; a fact closely related to its long-range character. Nevertheless, the procedure is applicable to such systems whenever the energy is below the three-body breakup threshold. For such cases one Lippmann-Schwinger equation is still sufficient to find solutions.

The “three-potential” integral equations have been solved previously by using a CS representation [5,6]. With n and l being the radial and orbital angular momentum quantum numbers respectively, the CS functions $|nl\rangle$ form a biorthonormal discrete basis in the two-body Hilbert space; the biorthogonal partner defined by $\langle r|nl\rangle = r^{-1}\langle r|nl\rangle$. Since the three-body Hilbert space is a direct sum of two-body Hilbert spaces, an appropriate basis in angular momentum representation is the direct product

$$|n\nu l\lambda\rangle_\alpha = [|nl\rangle_\alpha \otimes |\nu\lambda\rangle_\alpha], \quad (n, \nu = 0, 1, 2, \dots). \quad (16)$$

Here l and λ denote the angular momenta associated with the coordinates ξ and η , respectively. In this basis the completeness relation takes the form

$$\mathbf{1} = \lim_{N \rightarrow \infty} \sum_{n, \nu=0}^N |\widetilde{n\nu l\lambda}\rangle_\alpha \langle n\nu l\lambda| = \lim_{N \rightarrow \infty} \mathbf{1}_N^\alpha; \quad (17)$$

a sum over the angular momenta being assumed implicitly. Note that in the three-body Hilbert space, three equivalent bases belonging to fragmentation α , β and γ are possible.

To proceed, it is convenient to approximate Eqs. (15) by

$$|\psi_\beta^{(\pm)}\rangle = \delta_{\beta\alpha} |\Phi_\alpha^{(l)(\pm)}\rangle + G_\beta^{(l)} \mathbf{1}_N^\beta v_\beta^{(s)} \sum_{\gamma \neq \beta} \mathbf{1}_N^\gamma |\psi_\gamma^{(\pm)}\rangle, \quad (18)$$

with the short-range potential v_α^s in the three-body Hilbert space taken to have a separable form, viz.

$$v_\alpha^s \approx \sum_{n, \nu, n', \nu'=0}^N |\widetilde{n\nu l\lambda}\rangle_\alpha \underline{v}_{\alpha\beta}^s \langle n'\nu' l'\lambda'|, \quad (19)$$

where $\underline{v}_{\alpha\beta}^s = {}_\alpha \langle n\nu l\lambda | v_\alpha^s | n'\nu' l'\lambda' \rangle_\beta$. In Eq. (19) the ket and bra states are defined for different fragmentations, depending on the environment of the potential operators in the equations. A similar approximation is made on the potential U^α in Eqs. (14) and (13), with bases of the same fragmentation α applied on both sides of the operator. Thus, by truncating the short-range operators in Eqs. (15), (14) and (13), the set of linear integral equations reduces to an analogous set of linear algebraic equations with the operators replaced by their matrix representations. Calculation of $\underline{v}_{\alpha\beta}^s$ and of \underline{U}^α can be made as

shown previously [6]. A similar procedure enables calculation of the matrix elements $\underline{G}_\alpha = {}_\alpha \langle \widetilde{n\nu l\lambda} | \tilde{G}_\alpha | n'\nu' l'\lambda' \rangle_\alpha$ with three-body bound states [6]. The Green’s operator \tilde{G}_α is a resolvent of the sum of two commuting Hamiltonians, $h_{\xi_\alpha} = h_{\xi_\alpha}^0 + v_\alpha$ and $h_{\eta_\alpha} = h_{\eta_\alpha}^0 + u_\alpha^{(l)}$, which act in different two-body Hilbert spaces. Thus, using the convolution theorem [15], which is a direct consequence of Dunford’s operator calculus [16], the three-body Green’s operator \tilde{G}_α equates to a convolution integral of two-body Green’s operators, i.e.

$$\begin{aligned} \tilde{G}_\alpha(z) &= (z - h_{\xi_\alpha} - h_{\eta_\alpha})^{-1} \\ &= \frac{1}{2\pi i} \oint_C dz' g_{\xi_\alpha}(z - z') g_{\eta_\alpha}(z'), \end{aligned} \quad (20)$$

where $g_{\xi_\alpha}(z) = (z - h_{\xi_\alpha})^{-1}$ and $g_{\eta_\alpha}(z) = (z - h_{\eta_\alpha})^{-1}$. The contour C should be taken counterclockwise around the continuous spectrum of h_{η_α} so that g_{ξ_α} is analytic in the domain encircled by C . For bound-state energies the spectra of the two Green’s operators are well separated and this condition can be fulfilled easily [6]. Also, below breakup threshold, where the bound-state pole of g_{ξ_α} meets the continuous spectrum of g_{η_α} , contour integration can still be performed [5]. For other positive energy scattering problems, however, the continua overlap so the applied contours are not viable.

But there exists a contour which is valid for all z of physical interest. Besides positive real values of z that arise with scattering above the breakup threshold, this contour can deal with complex values of z having negative imaginary parts that are needed for resonant-state calculations. In this approach first one must shift the spectrum of g_{ξ_α} by taking $z = E + i\varepsilon$ with positive ε . By doing so, the two spectra are well separated and the spectrum of g_{η_α} can be encircled. Next the contour C is deformed analytically in such a way that the upper part descends to the second Riemann sheet of g_{η_α} , while the lower part of C can be detoured away from the cut [see Fig. 1]. The contour still encircles the branch cut singularity of g_{η_α} , but in the $\varepsilon \rightarrow 0$ limit it now avoids the singularities of g_{ξ_α} . Moreover, by continuing to negative values of ε , the branch cut and pole singularities of g_{ξ_α} move onto the second Riemann sheet of g_{η_α} and, at the same time, the branch cut of g_{η_α} moves onto the second Riemann sheet of g_{ξ_α} . Thus, the mathematical conditions for the contour integral representation of $\tilde{G}_\alpha(z)$ in Eq. (20) can be fulfilled for all energies. In this respect there is only a gradual difference between the bound- and resonant-state calculations and scattering ones below and above the breakup threshold.

The matrix elements \underline{G}_α can be cast in the form

$$\begin{aligned} \underline{G}_\alpha(z) &= \frac{1}{2\pi i} \oint_C dz' {}_\alpha \langle \widetilde{n\lambda} | g_{\xi_\alpha}(z - z') | \widetilde{n'l'} \rangle_\alpha \\ &\quad \times {}_\alpha \langle \widetilde{\nu\lambda} | g_{\eta_\alpha}(z') | \widetilde{\nu'l'} \rangle_\alpha. \end{aligned} \quad (21)$$

The matrix elements of the two-body Green's functions in the integrand are known for all complex energies from two-body state properties [17,18]. In this formalism the Faddeev components appear as linear combinations of functions

$$\langle \xi_\alpha \eta_\alpha | \psi_\alpha \rangle \sim \langle \xi_\alpha \eta_\alpha | \tilde{G}_\alpha(z) | \widetilde{n\nu l \lambda} \rangle_\alpha = \frac{1}{2\pi i} \oint_C dz' \langle \xi_\alpha | g_{\xi_\alpha}(z - z') | \widetilde{n l} \rangle_\alpha \langle \eta_\alpha | g_{\eta_\alpha}(z') | \widetilde{\nu \lambda} \rangle_\alpha, \quad (22)$$

which are convolution integrals of Coulomb-like functions [17].

In this paper I have shown that the set of Faddeev and Lippmann–Schwinger equations for the three-body Coulomb problem derived from the “three-potential” picture [5] possess compact kernels for all energies. I have found an analytic representation of the channel-distorted Coulomb Green's operators in terms of a convolution integral of two-body Green's operators. The method facilitates the solution of integral equations in which the exact bound- scattering- or resonant-state Coulomb asymptotics are automatically incorporated. Solution of these equations in a Coulomb–Sturmian space representation is most practical, as then there is an analytic representation of the terms in the contour integrals.

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- [13] J. Noble, Phys. Rev. **161**, 945 (1967).
- [14] S. P. Merkuriev, Ann. Phys. (N.Y.) **130**, 395 (1980); Acta Physica Austriaca, Supplementum XXIII, 65 (1981); L. D. Faddeev and S. P. Merkuriev, *Quantum Scattering Theory for Several Particle Systems*, (Kluwer, Dordrech), 1993.
- [15] L. Bianchi and L. Favella, Nuovo Cim. **6**, 6873 (1964).
- [16] N. Dunford and J. T. Schwartz, *Linear Operators I*, (Wiley Interscience, New York) 1958.
- [17] Z. Papp, J. Phys. A **20**, 153 (1987); Phys. Rev. C **38**, 2457 (1988); Phys. Rev. A **46**, 4437 (1992); Comp. Phys. Comm. **70**, 426, 435 (1992).
- [18] B. Kónya, G. Lévai, and Z. Papp, J. Math. Phys. **38**, 4832 (1997).

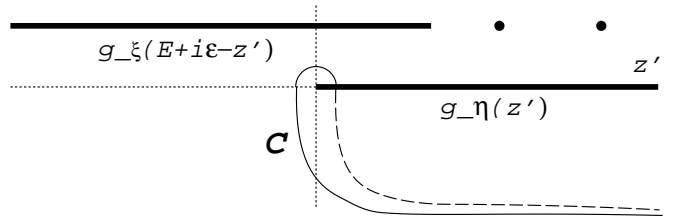


FIG. 1. Analytic structure of $g_{\xi_\alpha}(z - z') g_{\eta_\alpha}(z')$ as a function of z' with $z = E + i\varepsilon$, $E > 0$, $\varepsilon > 0$. The contour C encircles the continuous spectrum of h_{η_α} . A part of it, which goes on the second Riemann-sheet of h_{η_α} , is drawn by broken line.

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- [1] E. O. Alt and W. Sandhas, *Coulomb Interactions in Nuclear and Atomic Few-Body Collisions*, (eds. F. S. Levin and D. A. Micha, Plenum Press, New York), 1996, p1.
 - [2] J. L. Friar and G. L. Payne, *Coulomb Interactions in Nuclear and Atomic Few-Body Collisions*, (eds. F. S. Levin and D. A. Micha, Plenum Press, New York), 1996, p97.
 - [3] T. Kato, *Perturbation Theory for Linear Operators* (Springer, New York) 1966.
 - [4] Gy. Bencze, Lett. Nuovo Cim., **17**, 91 (1976); Gy. Bencze and H. Zankel, Phys. Lett. **82B**, 316 (1979).
 - [5] Z. Papp, Phys. Rev. C **55**, 1080 (1997).
 - [6] Z. Papp, and W. Plessas, Phys. Rev. C **54**, 50 (1996).
 - [7] Z. Papp, Few-Body Systems, (in print), (physics/9702001).
 - [8] C. R. Chen, G. L. Payne, J. L. Friar, and B. F. Gibson, Phys. Rev. C **39**, 1261 (1989).
 - [9] J. Dollard, J. Math. Phys. **5**, 729 (1964); **14**, 708 (1973).
 - [10] J. R. Taylor, *Scattering Theory* (Wiley, New York), 1972.
 - [11] W. O. Amrein, J. M. Jauch, and K. B. Sinha, *Scattering Theory in Quantum Mechanics*, (Benjamin, Reading) 1977.
 - [12] W. Sandhas, *Few-Body Nuclear Physics*, (IAEA Vienna, 1978), p3.